10563975

NEWS IPC8   For general information regarding STN implementation of IPC 8
NEWS X25   X.25 communication option no longer available

Enter NEWS followed by the item number or name to see news on that
specific topic.

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  of commercial gateways or other similar uses is prohibited and may
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* * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:50:09 ON 21 FEB 2007

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                              ENTRY   SESSION
FULL ESTIMATED COST   0.21   0.21

FILE 'REGISTRY' ENTERED AT 09:50:16 ON 21 FEB 2007
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DICTIONARY FILE UPDATES: 19 FEB 2007   HIGHEST RN 921921-74-6

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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
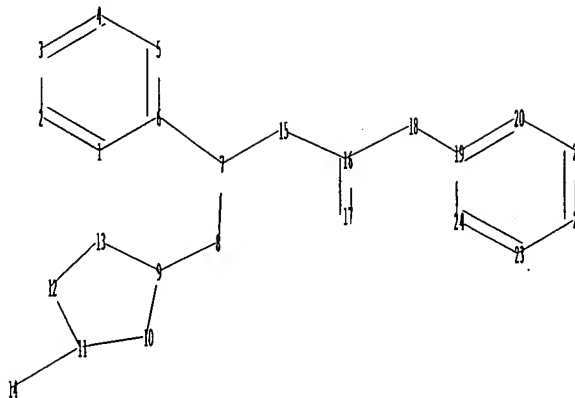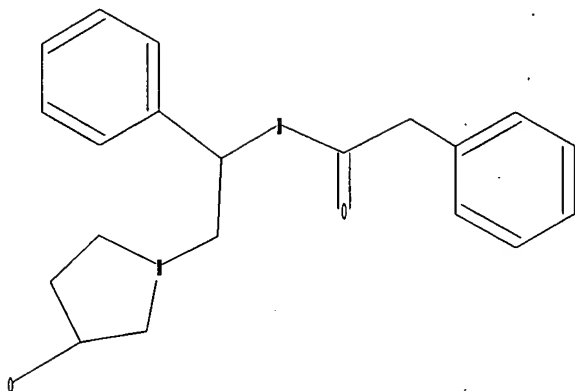on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10563975.str

Karen Cheng

broadest search

chain nodes :
7 8 14 15 16 17 18
ring nodes :
1 2 3 4 5 6 9 10 11 12 13 19 20 21 22 23 24
chain bonds :
6-7 7-8 7-15 8-9 11-14 15-16 16-17 16-18 18-19
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 9-10 9-13 10-11 11-12 12-13 19-20 19-24 20-21
21-22 22-23 23-24
exact/norm bonds :
7-15 8-9 9-10 9-13 11-14 15-16 16-17
exact bonds :
6-7 7-8 10-11 11-12 12-13 16-18 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 19-20 19-24 20-21 21-22 22-23 23-24
isolated ring systems :
containing 1 : 9 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom

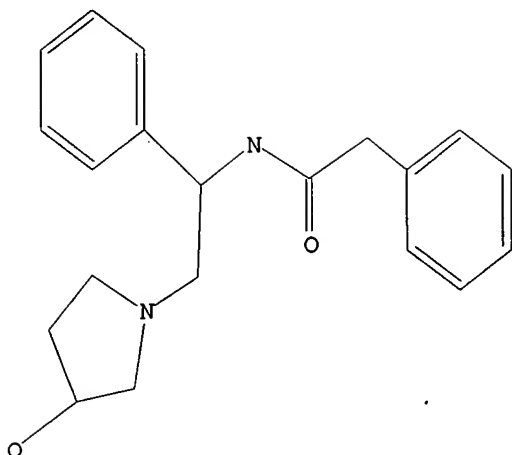L1   STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1   STR

Karen Cheng

10563975

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 09:50:39 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   1304 TO ITERATE

100.0% PROCESSED   1304 ITERATIONS   359 ANSWERS
SEARCH TIME: 00.00.01

L2   359 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                               ENTRY   SESSION
FULL ESTIMATED COST   172.10   172.31

FILE 'CAPLUS' ENTERED AT 09:50:48 ON 21 FEB 2007
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FILE LAST UPDATED: 19 Feb 2007   (20070219/ED)

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http://www.cas.org/infopolicy.html

=> s l2
L3   83 L2

=> fil stng
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                        ENTRY   SESSION
FULL ESTIMATED COST   0.47   172.78

FILE 'STNGUIDE' ENTERED AT 09:50:53 ON 21 FEB 2007
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FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Feb 16, 2007 (20070216/UP).

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                        ENTRY   SESSION
FULL ESTIMATED COST   0.18   172.96

FILE 'REGISTRY' ENTERED AT 09:52:44 ON 21 FEB 2007
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DICTIONARY FILE UPDATES: 19 FEB 2007   HIGHEST RN 921921-74-6

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predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
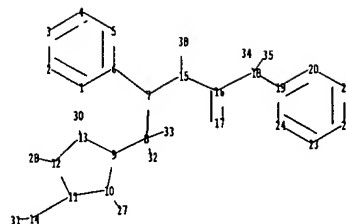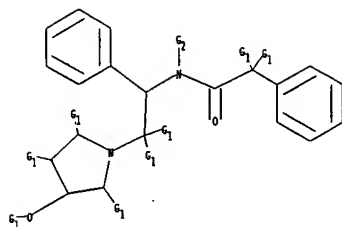on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10563975a.str...

Karen Cheng

limit H substituents to H's, Me

chain nodes :
7 8   14   15   16   17   18   27   28   30   31   32   33   34   35   38
ring nodes :
1 2   3   4   5   6   9   10   11   12   13   19   20   21   22   23   24
chain bonds :
6-7   7-8   7-15   8-9   8-32   8-33   10-27   11-14   12-28   13-30   14-31   15-16   15-38
16-17   16-18   18-19   18-34   18-35
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   9-10   9-13   10-11   11-12   12-13   19-20   19-24   20-21
21-22   22-23   23-24
exact/norm bonds :
7-15   8-9   8-32   8-33   9-10   9-13   10-27   11-14   12-28   13-30   14-31   15-16   15-38
16-17   18-34   18-35
exact bonds :
6-7   7-8   10-11   11-12   12-13   16-18   18-19
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   19-20   19-24   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 9 :

G1:H,CH3

G2:H,Ak

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
19:Atom   20:Atom   21:Atom   22:Atom   23:Atom   24:Atom   27:CLASS   28:CLASS   30:CLASS ...
31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   38:CLASS

L4   STRUCTURE UPLOADED

Karen Cheng

10563975

```
=> d his

        (FILE 'HOME' ENTERED AT 09:50:09 ON 21 FEB 2007)

        FILE 'REGISTRY' ENTERED AT 09:50:16 ON 21 FEB 2007
L1              .    STRUCTURE UPLOADED
L2           359 S L1 FULL

        FILE 'CAPLUS' ENTERED AT 09:50:48 ON 21 FEB 2007
L3            83 S L2

        FILE 'STNGUIDE' ENTERED AT 09:50:53 ON 21 FEB 2007

        FILE 'REGISTRY' ENTERED AT 09:52:44 ON 21 FEB 2007
L4              STRUCTURE UPLOADED

=> s l4 full sub=l2
FULL SUBSET SEARCH INITIATED 09:53:26 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -      359 TO ITERATE

100.0% PROCESSED      359 ITERATIONS                        253 ANSWERS
SEARCH TIME: 00.00.01

L5         253 SEA SUB=L2 SSS FUL L4

=> fil caplus
COST IN U.S. DOLLARS                         SINCE FILE        TOTAL
                                               ENTRY          SESSION
FULL ESTIMATED COST                           41.10          214.06

FILE 'CAPLUS' ENTERED AT 09:53:35 ON 21 FEB 2007
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FILE LAST UPDATED: 19 Feb 2007   (20070219/ED)
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```
=> s l5
L6          78 L5

=> fil stng
```

Karen Cheng

10563975

COST IN U.S. DOLLARS		SINCE FILE	TOTAL
		ENTRY	SESSION
FULL ESTIMATED COST		0.47	214.53

FILE 'STNGUIDE' ENTERED AT 09:53:41 ON 21 FEB 2007
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=> fil reg
COST IN U.S. DOLLARS		SINCE FILE	TOTAL
		ENTRY	SESSION
FULL ESTIMATED COST		0.42	214.95

FILE 'REGISTRY' ENTERED AT 09:57:36 ON 21 FEB 2007
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DICTIONARY FILE UPDATES: 19 FEB 2007   HIGHEST RN 921921-74-6

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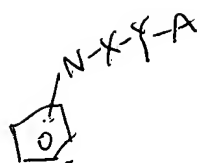   conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10563975b.str
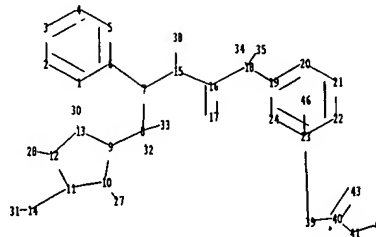
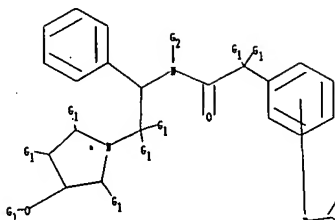Karen Cheng

add -N substituent off benzene ring.

X = CO. or CS

Y = O, NH, CH2

A = Cy

Cy = ring systems.

chain nodes :
7   8   14 15 16 17 18 27 28 30 31 32 33 34 35 38 39 40 41 42 43
ring nodes :
1   2   3   4   5   6   9   10 11 12 13 19 20 21 22 23 24
chain bonds :
6-7   7-8   7-15   8-9   8-32   8-33   10-27   11-14   12-28   13-30   14-31   15-16   15-38
16-17   16-18   18-19   18-34   18-35   39-40   40-41   40-43   41-42
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   9-10   9-13   10-11   11-12   12-13   19-20   19-24   20-21
21-22   22-23   23-24
exact/norm bonds :
7-15   8-9   8-32   8-33   9-10   9-13   10-27   11-14   12-28   13-30   14-31   15-16   15-38
16-17   18-34   18-35   39-40   40-41   40-43   41-42
exact bonds :
6-7   7-8   10-11   11-12   12-13   16-18   18-19
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   19-20   19-24   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 9 :

G1:H,CH3

G2:H,Ak

G3:C,O,N

G4:O,S

Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
19:Atom   20:Atom   21:Atom   22:Atom   23:Atom   24:Atom   27:CLASS   28:CLASS   30:CLASS
31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   38:CLASS   39:CLASS   40:CLASS
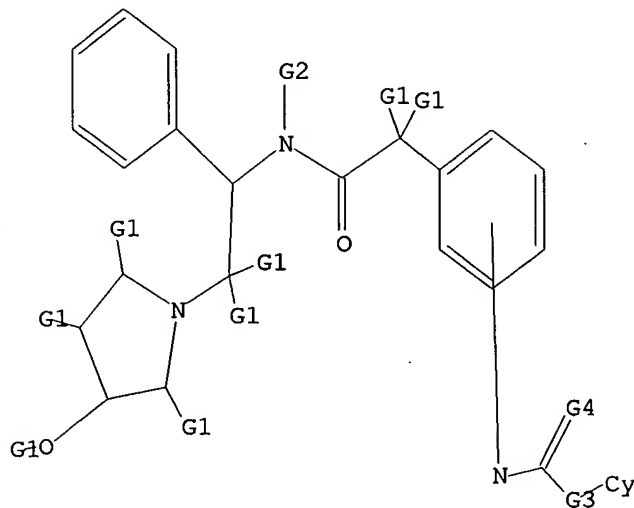41:CLASS   42:Atom   43:CLASS   46:Atom

Karen Cheng

L7   STRUCTURE UPLOADED

=> d
L7 HAS NO ANSWERS
L7   STR

G1 H,Me

G2 H,Ak

G3 C,O,N

G4 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l7 full
FULL SEARCH INITIATED 09:58:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   793 TO ITERATE

100.0% PROCESSED   793 ITERATIONS   12 ANSWERS
SEARCH TIME: 00.00.01

L8   12 SEA SSS FUL L7

=> fil caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                            ENTRY   SESSION
FULL ESTIMATED COST   172.10   387.05

FILE 'CAPLUS' ENTERED AT 09:58:09 ON 21 FEB 2007
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=> s l8
L9   1 L8

=> d ibib abs hitstr tot

Karen Cheng

10563975

=> fil reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                        ENTRY   SESSION
FULL ESTIMATED COST   5.74   570.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                        ENTRY   SESSION
CA SUBSCRIBER PRICE   -0.78   -1.56

FILE 'REGISTRY' ENTERED AT 10:00:20 ON 21 FEB 2007
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DICTIONARY FILE UPDATES: 19 FEB 2007   HIGHEST RN 921921-74-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006
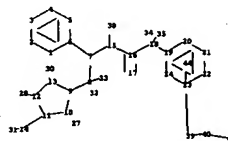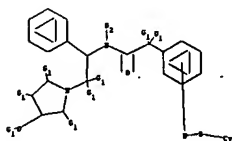
   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10563975d.str

Karen Cheng

```
chain nodes :
7   8   14  15  16  17  18  27  28  30  31  32  33  34  35  38  39  40  41
ring nodes :
1   2   3   4   5   6   9   10  11  12  13  19  20  21  22  23  24
chain bonds :
6-7   7-8   7-15   8-9   8-32   8-33   10-27   11-14   12-28   13-30   14-31   15-16   15-38
16-17   16-18   18-19   18-34   18-35   39-40   40-41
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   9-10   9-13   10-11   11-12   12-13   19-20   19-24   20-21
21-22   22-23   23-24
exact/norm bonds :
7-15   8-9   8-32   8-33   9-10   9-13   10-27   11-14   12-28   13-30   14-31   15-16   15-38
16-17   18-34   18-35   39-40   40-41
exact bonds :
6-7   7-8   10-11   11-12   12-13   16-18   18-19
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   19-20   19-24   20-21   21-22   22-23   23-24
isolated ring systems :
containing 1 : 9 :
```

G1:H,CH3

G2:H,Ak

G3:C,O,N

G4:O,S

```
Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:CLASS   8:CLASS   9:Atom   10:Atom
11:Atom   12:Atom   13:Atom   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
19:Atom   20:Atom   21:Atom   22:Atom   23:Atom   24:Atom   27:CLASS   28:CLASS   30:CLASS
31:CLASS   32:CLASS   33:CLASS   34:CLASS   35:CLASS   38:CLASS   39:CLASS   40:CLASS
41:Atom   44:Atom
```
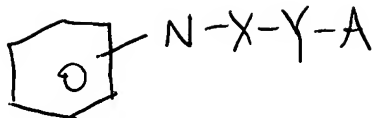
L13   STRUCTURE UPLOADED
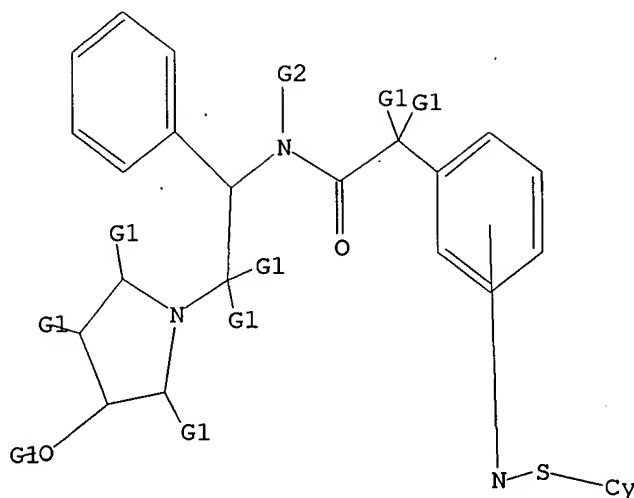
=> d
L13 HAS NO ANSWERS
L13   STR

Karen Cheng

N—X—Y—A

$X = SO_2$

Y = single bond

A = Cy = ring systems

G1 H,Me

G2 H,Ak

G3 C,O,N

G4 O,S

Structure attributes must be viewed using STN Express query preparation.

```
=> d his

    (FILE 'HOME' ENTERED AT 09:50:09 ON 21 FEB 2007)

    FILE 'REGISTRY' ENTERED AT 09:50:16 ON 21 FEB 2007
L1              STRUCTURE UPLOADED
L2        359 S L1 FULL

    FILE 'CAPLUS' ENTERED AT 09:50:48 ON 21 FEB 2007
L3         83 S L2

    FILE 'STNGUIDE' ENTERED AT 09:50:53 ON 21 FEB 2007

    FILE 'REGISTRY' ENTERED AT 09:52:44 ON 21 FEB 2007
L4              STRUCTURE UPLOADED
L5        253 S L4 FULL    SUB=L2

    FILE 'CAPLUS' ENTERED AT 09:53:35 ON 21 FEB 2007
L6         78 S L5

    FILE 'STNGUIDE' ENTERED AT 09:53:41 ON 21 FEB 2007

    FILE 'REGISTRY' ENTERED AT 09:57:36 ON 21 FEB 2007
L7              STRUCTURE UPLOADED
L8         12 S L7 FULL
```

Karen Cheng

10563975

```
      FILE 'CAPLUS' ENTERED AT 09:58:09 ON 21 FEB 2007
L9          1 S L8

      FILE 'STNGUIDE' ENTERED AT 09:58:38 ON 21 FEB 2007

      FILE 'REGISTRY' ENTERED AT 09:59:29 ON 21 FEB 2007
L10           STRUCTURE UPLOADED
L11          4 S L10 FULL

      FILE 'CAPLUS' ENTERED AT 10:00:04 ON 21 FEB 2007
L12          1 S L11

      FILE 'REGISTRY' ENTERED AT 10:00:20 ON 21 FEB 2007
L13           STRUCTURE UPLOADED

=> s l13 full sub=l5
FULL SUBSET SEARCH INITIATED 10:01:38 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED -        76 TO ITERATE

100.0% PROCESSED       76 ITERATIONS                25 ANSWERS
SEARCH TIME: 00.00.01

L14          25 SEA SUB=L5 SSS FUL L13
```

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	41.55	612.24

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.56

FILE 'CAPLUS' ENTERED AT 10:01:43 ON 21 FEB 2007
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10563975

```
=> s l14
L15              1 L14

=> d ibib abs hitstr tot
```

Karen Cheng